



UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
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OFFICE OF PREVENTION, PESTICIDES AND
TOXIC SUBSTANCES

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MEMORANDUM

SUBJECT: Estimated Drinking Water Concentrations for Metam Sodium and its Metabolite Methyl isothiocyanate for Application on Florida Tomato

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This memo presents a Tier II Estimated Drinking Water Concentrations (EDWCs) for metam sodium (sodium N-methyldithiocarbamate, an active ingredient for fumigants) and its metabolite methyl isothiocyanate (MITC), based on a maximum application rate of 320 lbs. a.i./Acre. The models, PRZM/EXAMS and SCIGROW were used in estimating EDWCs in surface water and groundwater, respectively. The acute concentrations in surface water are 0.03 : g/L for metam sodium and 73.22 : g/L for MITC. The cancer chronic concentrations are 2.99 : g/L for MITC and negligible (#0.001 : g/L) for metam sodium using the Florida tomato scenario. These values represent the mean value over a 30-year period. Several other scenarios (onion, strawberry, and turf) were also investigated but gave consistently lower EDWCs (results not reported here). The SCIGROW generated EDWCs for tomato 0.13: g/L for metam sodium and 0.72 : g/L for MITC, which are recommended to use for both acute and chronic

exposers. The results are presented in Table 1.

Table 1. Estimated Drinking Water Concentrations (EDWC's) in surface water and Groundwater

Chemical	Surface Water ($\mu\text{g/L}$)			Groundwater ($\mu\text{g/L}$)
	Acute	Non-cancer chronic	cancer chronic	
Florida Tomato				
Metam Sodium	0.03	0.0	0.0	0.13*
MITC	73.22	0.53	2.99	0.72*

* Recommended EDWCs values for acute and chronic for groundwater

1.0 ESTIMATION OF SURFACE WATER AND GROUNDWATER EXPOSURE CONCENTRATIONS

The maximum application rates and relevant environmental fate parameters for metam sodium and MITC were used in the two screening models PRZM/EXAMS and SCIGROW for EDWCs in surface water and groundwater, respectively. In absence of environmental fate data of MITC, EFED used selected environmental fate data from open literature to estimate EDWCs. Since MITC is a volatile compound, additional input parameters like DAIR (vapor phase diffusion coefficient) and ENPY (enthalpy of vaporization) were activated during the PRZM-EXAMS simulation. The outputs of the two screening models represent estimates of the concentrations that might be found in surface water and groundwater due to the use of metam sodium on Florida tomato.

2.0 Background Information on PRZM/EXAMS

The linked PRZM (3.12) and EXAMS (2.98.5) model (PRZM/EXAMS) is typically used by EFED in estimating pesticides concentrations in surface waters. PRZM is employed to evaluate runoff loading to a receiving surface water body. As soon as the pesticide residues reaches the surface water, EXAMS uses algorithms to the pesticides concentrations by taken into account different dissipation mechanism in the aqueous and sediment phases.

PRZM (3.12) is a one-dimensional finite-difference modeling system that was originally developed to model nitrogen soil kinetic processes and groundwater environment. It was later enhanced to expand its capability to predict pesticides transport and transformation down through the crop zone and saturated zone. The expanded capabilities cover additional phenomena such as soil temperature simulation, microbial transformation, vapor phase transport in soils, volatilization, irrigation simulation, and a method of characteristics (MOC) algorithm to eliminate numerical dispersion. The model can also simulate the fate of two parent and two daughter products and often used in evaluating leaching and runoff.

EXAMS (2.98.5) is a model that has a set of process modules that link fundamental chemical properties to limnological processes that control the kinetics and transport of chemicals in aquatic systems. It provides facilities for steady state or long-term evaluation of chronic chemical discharges, initial-value approaches for studying short-term contaminant releases, and full kinetic simulations that allow for monthly variation in mean climatological factors, and changes in contaminant loadings on daily time scales. It is fairly and relatively complex model that requires more input variables, ranging from hydro-geological and weather data to pesticide physicochemical properties, mobility coefficients, and degradation rate constants in the aqueous and sediment phases.

3.0 Background Information on SCI-GROW

SCIGROW is a regression-based model that provides a groundwater screening exposure value to be used in determining the potential risk to human health from drinking water contaminated with the pesticide. Since the SCI-GROW concentrations are likely to be approached in only very small percentage of drinking water sources (i.e. highly vulnerable aquifers), it is not appropriate to use SCI-GROW for national or regional exposure estimates.

SCIGROW estimates likely groundwater concentrations if the pesticide is used at the maximum allowable rate in areas where groundwater is exceptionally vulnerable to contamination. In most cases, a large majority of the use area will have groundwater that is less vulnerable to contamination than the areas used to derive the SCIGROW estimate.

4.0 Modeling Inputs and Results:

Tables 2 and 3 summarize the metam sodium input values used in the model runs for PRZM (3.12), EXAMS 2.98.5) and SCIGROW, respectively. Tables 4 and 5 summarize the MITC input values used in the model runs for PRZM (3.12), EXAMS 2.98.5) and SCIGROW, respectively. Application information is included in Table 2 and 4. Modeling results are presented in Table 1 for PRZM (3.12)/EXAMS (2.98.5) and SCIGROW. This memo also contains the copies of the printouts generated from the PRZM/EXAMS, SCIGROW, and EPISUITE runs.

Table 2. PRZM/EXAM Input Parameters for Metam Sodium

Parameters	Values & Units	Sources
Molecular Weight	129.2 g Mole ⁻¹	Product Chemistry
Vapor Pressure 25°C	Non volatile	Agrochemical Handbook
Water Solubility @ pH 7.0 and 25°C	722g L ⁻¹	Product Chemistry
Hydrolysis Half-Life (pH 5)	2.0 Days	MRID 41631101
Hydrolysis Half-Life (pH 7)	2.0 Days	MRID 41631101
Hydrolysis Half-Life (pH 9)	9.0 Days	MRID 41631101

Table 2. PRZM/EXAM Input Parameters for Metam Sodium

Parameters	Values & Units	Sources
Aerobic Soil Metabolism $t_{1/2}$,	0.06 Days *	MRID 40198502
Aerobic Aquatic metabolism: for entire sediment/water system	0.12 **	EFED Guideline
Aqueous Photolysis	0.02 Day	MRID 41517701
Soil Water Partition Coefficient	4.038 L Kg ⁻¹	EPISUITE***
Pesticide is Wetted-In	No	Product Label
Crop Management-Tomato		
Pesticide Frequency & application rates (lb a.i./A)	320.0	Registrant Provided
First Application Date	April 15	Registrant Provided
Application interval	None	Registrant Provided
Application Method	Ground Injection	Registrant Provided
Spray Efficiency	100%	EFED
Spray Drift (Index Res. Scenario)	None	EFED

* = Due to one reported half-life, input half-life was multiplied by 3 according to Guidance for selecting input parameters in modeling for environmental fate and transport of pesticides. Version II. December 4, 2001.

**= In absence of aerobic aquatic metabolism half-life, the reported half-lives of aerobic soil metabolism multiplied by 2 according to Guidance for selecting input parameters in modeling for environmental fate and transport of pesticides. Version II. December 4, 2001.

*** = The EPI (Estimation Program Interface) SuiteTM is a Windows® based suite of physical/chemical property and environmental fate estimation models developed by the EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation SRC. http://www.epa.gov/opptintr/exposure/docs/updates_episodes_v3.11.htm

Table 3. Environmental Fate Input Parameters for Metam Sodium in SCIGROW.

Parameter	Values & Units	Reference
Organic carbon partition coefficient (K _{OC})	4.038 mL/g	EPISUITE*
Aerobic soil metabolism half-life (days)	0.06 Days	MRID 40198502

* = The EPI (Estimation Program Interface) SuiteTM is a Windows® based suite of physical/chemical property and environmental fate estimation models developed by the EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation SRC. http://www.epa.gov/opptintr/exposure/docs/updates_episodes_v3.11.htm

Table 4. PRZM/EXAM Input Parameters for MITC, a metam sodium Metabolite

Parameters	Values & Units	Sources
Molecular Weight	73.12g Mole ⁻¹	Product Chemistry
Vapor Pressure 25°C	19 mm Hg	CDPR, 2002
Water Solubility @ pH 7.0 and 25°C	7600 mg L ⁻¹	Product Chemistry
Vapor Phase Diffusion Coefficient (DAIR)	4300 cm ² day ⁻¹ (Default)	Carsel et al., 1997
Enthalpy of Vaporization	20 kcal mole ⁻¹ (Default)	Carsel et al., 1997
Hydrolysis Half-Life (pH 7)	20.4	CDPR, 2002
Aerobic Soil Metabolism t _{1/2} ,	6.01 Days (mean value)	Gerstl et at., 1977
Aerobic Aquatic metabolism: for entire sediment/water system	12.02 [†]	EFED Guideline
Anaerobic aquatic metabolism	Stable	MRID 439084-26
Aqueous Photolysis	51.6 Day	CDPR, 2002
Soil Water Partition Coefficient	0.26 L Kg ⁻¹ (Mean K _d)	Gerstl et at., 1977

Crop Management- Florida Tomato

Pesticide application frequency and rate	150.3 (lb a.i./A) [‡]	Estimated
Application Date	April 15	Registrant Provided
Application Method	Ground	EFED Guideline
Spray Efficiency	100%	EFED Guideline

[†] = In absence of aerobic aquatic half-life, the reported half-lives of aerobic soil metabolism multiplied by 2 according to Guidance for selecting input parameters in modeling for environmental fate and transport of pesticides. Version II. December 4, 2001.

[‡] = Metam sodium application rate x [(0.83, the maximum conversion rate from the degradation of metam sodium to MITC in the hydrolysis study) x (0.57, the molecular weight ratio of MITC to metam Sodium)]

Table 5. Environmental Fate Input Parameters for MITC in SCIGROW.

Parameter	Value	Reference
Organic carbon partition coefficient (K _{OC})	14.86 (Median value)	Table 6.
Aerobic soil metabolism half-life (days)	4.8 (Median value)	Gerstl et at., 1977

Table 6. Estimation of Koc[‡]

Soil	Organic matter (%)	Organic Carbon (%)	Kd (mL/g)	Koc (mL/g)
Mivtachim	0.45	0.26	0.012	4.60
Gilat	0.5	0.29	0.045	15.52

Golan	4.98	2.89	0.41	14.19
Har Baroan	4.10	2.38	0.57	23.97
Median Value				14.86

[‡] Gerstl et al., 1977

PRZM/EXAMS Model Output for Metam Sodium on Florida Tomato

Chemical: MetamSodium

PRZM environment: FLtomatoC.txt

EXAMS environment: ir298.exv

Metfile: w12844.dvf

Water segment concentrations (ppb)						
Year	Peak	96 hr	21 Day	60 Day	90 Day	Yearly
1961	0.00	0.00	0.00	0.00	0.00	0.00
1962	0.00	0.00	0.00	0.00	0.00	0.00
1963	0.00	0.00	0.00	0.00	0.00	0.00
1964	0.04	0.01	0.00	0.00	0.00	0.00
1965	0.00	0.00	0.00	0.00	0.00	0.00
1966	0.00	0.00	0.00	0.00	0.00	0.00
1967	0.00	0.00	0.00	0.00	0.00	0.00
1968	0.00	0.00	0.00	0.00	0.00	0.00
1969	0.00	0.00	0.00	0.00	0.00	0.00
1970	0.00	0.00	0.00	0.00	0.00	0.00
1971	0.00	0.00	0.00	0.00	0.00	0.00
1972	0.00	0.00	0.00	0.00	0.00	0.00
1973	0.00	0.00	0.00	0.00	0.00	0.00
1974	0.00	0.00	0.00	0.00	0.00	0.00
1975	0.00	0.00	0.00	0.00	0.00	0.00
1976	0.00	0.00	0.00	0.00	0.00	0.00
1977	0.00	0.00	0.00	0.00	0.00	0.00
1978	0.00	0.00	0.00	0.00	0.00	0.00
1979	0.00	0.00	0.00	0.00	0.00	0.00
1980	0.00	0.00	0.00	0.00	0.00	0.00
1981	0.00	0.00	0.00	0.00	0.00	0.00
1982	0.00	0.00	0.00	0.00	0.00	0.00
1983	0.00	0.00	0.00	0.00	0.00	0.00
1984	0.00	0.00	0.00	0.00	0.00	0.00
1985	2.06	0.26	0.05	0.02	0.01	0.00
1986	0.00	0.00	0.00	0.00	0.00	0.00
1987	0.00	0.00	0.00	0.00	0.00	0.00
1988	0.00	0.00	0.00	0.00	0.00	0.00
1989	13.55	1.70	0.32	0.11	0.08	0.02
1990	0.00	0.00	0.00	0.00	0.00	0.00

Sorted results

Prob.	Peak	96 hr	21 Day	60 Day	90 Day	Yearly
0.03	13.55	1.70	0.32	0.11	0.08	0.02
0.06	2.06	0.26	0.05	0.02	0.01	0.00
0.10	0.04	0.01	0.00	0.00	0.00	0.00
0.13	0.00	0.00	0.00	0.00	0.00	0.00
0.16	0.00	0.00	0.00	0.00	0.00	0.00
0.19	0.00	0.00	0.00	0.00	0.00	0.00
0.23	0.00	0.00	0.00	0.00	0.00	0.00
0.26	0.00	0.00	0.00	0.00	0.00	0.00
0.29	0.00	0.00	0.00	0.00	0.00	0.00
0.32	0.00	0.00	0.00	0.00	0.00	0.00

0.35	0.00	0.00	0.00	0.00	0.00	0.00
0.39	0.00	0.00	0.00	0.00	0.00	0.00
0.42	0.00	0.00	0.00	0.00	0.00	0.00
0.45	0.00	0.00	0.00	0.00	0.00	0.00
0.48	0.00	0.00	0.00	0.00	0.00	0.00
0.52	0.00	0.00	0.00	0.00	0.00	0.00
0.55	0.00	0.00	0.00	0.00	0.00	0.00
0.58	0.00	0.00	0.00	0.00	0.00	0.00
0.61	0.00	0.00	0.00	0.00	0.00	0.00
0.65	0.00	0.00	0.00	0.00	0.00	0.00
0.68	0.00	0.00	0.00	0.00	0.00	0.00
0.71	0.00	0.00	0.00	0.00	0.00	0.00
0.74	0.00	0.00	0.00	0.00	0.00	0.00
0.77	0.00	0.00	0.00	0.00	0.00	0.00
0.81	0.00	0.00	0.00	0.00	0.00	0.00
0.84	0.00	0.00	0.00	0.00	0.00	0.00
0.87	0.00	0.00	0.00	0.00	0.00	0.00
0.90	0.00	0.00	0.00	0.00	0.00	0.00
0.94	0.00	0.00	0.00	0.00	0.00	0.00
0.97	0.00	0.00	0.00	0.00	0.00	0.00
0.1	0.04	0.00	0.00	0.00	0.00	0.00

Average of yearly averages:0.00

Estimated Drinking Water Concentration (EDWC)

$$\begin{aligned} \text{Acute EEC} &= (1/10 \text{ peak value})(\text{ percent crop area}) \\ &(0.04 : \text{g/L})(0.87) = 0.03 : \text{g/L} \end{aligned}$$

$$\begin{aligned} \text{Non-cancer Chronic EEC} &= (1/10 \text{ yearly value})(\text{percent area area}) \\ &0.00 : \text{g/L} \end{aligned}$$

$$\begin{aligned} \text{Cancer chronic EEC} &= (\text{Mean of annual value})(\text{percent crop area}) \\ &0.00 : \text{g/L} \end{aligned}$$

PRZM/EXAMS Model Output for MITC on Florida Tomato

Chemical: MITC

PRZM environment: FLtomatoC.txt

EXAMS environment: ir298.exv

Metfile: w12844.dvf

Year	Water segment concentrations (ppb)					
	Peak	96 hr	21 Day	60 Day	90 Day	Yearly
1961	0.03	0.02	0.01	0.00	0.00	0.00
1962	0.79	0.46	0.12	0.04	0.03	0.01
1963	2.97	1.50	0.35	0.12	0.08	0.02
1964	84.34	39.73	10.48	3.71	2.48	0.61
1965	0.02	0.01	0.00	0.00	0.00	0.00
1966	0.14	0.07	0.02	0.01	0.00	0.00
1967	0.00	0.00	0.00	0.00	0.00	0.00

1968	0.11	0.06	0.03	0.01	0.01	0.00
1969	1.50	0.80	0.19	0.07	0.04	0.01
1970	0.03	0.01	0.00	0.00	0.00	0.00
1971	0.81	0.39	0.13	0.05	0.03	0.01
1972	82.58	40.54	9.99	3.52	2.35	0.58
1973	0.58	0.28	0.07	0.02	0.02	0.00
1974	0.02	0.01	0.00	0.00	0.00	0.00
1975	0.03	0.02	0.01	0.00	0.00	0.00
1976	0.30	0.19	0.06	0.02	0.02	0.00
1977	3.52	1.65	0.41	0.15	0.10	0.02
1978	3.07	1.52	0.40	0.14	0.09	0.02
1979	28.49	13.54	3.39	1.19	0.79	0.20
1980	25.71	12.90	3.07	1.08	0.72	0.18
1981	0.13	0.06	0.02	0.01	0.00	0.00
1982	13.26	7.43	1.87	0.65	0.44	0.11
1983	0.01	0.01	0.00	0.00	0.00	0.00
1984	0.04	0.02	0.01	0.00	0.00	0.00
1985	3450.00	1720.00	408.00	143.00	95.28	23.49
1986	0.03	0.02	0.00	0.00	0.00	0.00
1987	0.43	0.20	0.08	0.03	0.02	0.00
1988	2.84	1.40	0.33	0.12	0.08	0.02
1989	11600.00	5780.00	1350.00	473.00	315.00	77.79
1990	4.24	2.04	0.48	0.17	0.11	0.03

Sorted results

Prob.	Peak	96 hr	21 Day	60 Day	90 Day	Yearly
0.03	11600.00	5780.00	1350.00	473.00	315.00	77.79
0.06	3450.00	1720.00	408.00	143.00	95.28	23.49
0.10	84.34	40.54	10.48	3.71	2.48	0.61
0.13	82.58	39.73	9.99	3.52	2.35	0.58
0.16	28.49	13.54	3.39	1.19	0.79	0.20
0.19	25.71	12.90	3.07	1.08	0.72	0.18
0.23	13.26	7.43	1.87	0.65	0.44	0.11
0.26	4.24	2.04	0.48	0.17	0.11	0.03
0.29	3.52	1.65	0.41	0.15	0.10	0.02
0.32	3.07	1.52	0.40	0.14	0.09	0.02
0.35	2.97	1.50	0.35	0.12	0.08	0.02
0.39	2.84	1.40	0.33	0.12	0.08	0.02
0.42	1.50	0.80	0.19	0.07	0.04	0.01
0.45	0.81	0.46	0.13	0.05	0.03	0.01
0.48	0.79	0.39	0.12	0.04	0.03	0.01
0.52	0.58	0.28	0.08	0.03	0.02	0.00
0.55	0.43	0.20	0.07	0.02	0.02	0.00
0.58	0.30	0.19	0.06	0.02	0.02	0.00
0.61	0.14	0.07	0.03	0.01	0.01	0.00
0.65	0.13	0.06	0.02	0.01	0.00	0.00
0.68	0.11	0.06	0.02	0.01	0.00	0.00
0.71	0.04	0.02	0.01	0.00	0.00	0.00
0.74	0.03	0.02	0.01	0.00	0.00	0.00
0.77	0.03	0.02	0.01	0.00	0.00	0.00

0.81	0.03	0.02	0.00	0.00	0.00	0.00
0.84	0.03	0.01	0.00	0.00	0.00	0.00
0.87	0.02	0.01	0.00	0.00	0.00	0.00
0.90	0.02	0.01	0.00	0.00	0.00	0.00
0.94	0.01	0.01	0.00	0.00	0.00	0.00
0.97	0.00	0.00	0.00	0.00	0.00	0.00
0.10	84.16	40.46	10.43	3.69	2.46	0.61
Average of yearly averages:3.44						

Estimated Drinking Water Concentration (EDWC)

Acute EEC = (1/10 peak value)(percent crop area)

$$(84.16 : \text{g/L})(0.87) = 73.22 : \text{g/L}$$

Non-cancer Chronic EEC =(1/10 yearly value)(percent area area)

$$(0.61 : \text{g/L})(0.87) = 0.53 : \text{g/L}$$

Cancer chronic EEC = (Mean of annual value)(percent crop area)

$$(3.44 : \text{g/L})(0.87) = 2.99 : \text{g/L}$$

SCIGROW Model Output for Metam Sodium on Florida Tomato

SCIGROW
VERSION 2.3
ENVIRONMENTAL FATE AND EFFECTS DIVISION
U.S. ENVIRONMENTAL PROTECTION AGENCY
SCREENING MODEL FOR AQUATIC PESTICIDE EXPOSURE

SciGrow version 2.3
chemical:Metam Sodium
time is 9/10/2003 12: 5: 0

Application rate (lb/acre)	Number of applications	Total Use (lb/acre/yr)	Koc (ml/g)	Soil Aerobic metabolism (days)
320.000	1.0	320.000	4.04E+00	0.1

groundwater screening cond (ppb) = 1.25E-01

SCIGROW Model Output for MITC on Florida Tomato

SCIGROW
VERSION 2.3
ENVIRONMENTAL FATE AND EFFECTS DIVISION
OFFICE OF PESTICIDE PROGRAMS
U.S. ENVIRONMENTAL PROTECTION AGENCY
SCREENING MODEL FOR AQUATIC PESTICIDE EXPOSURE

SciGrow version 2.3
chemical:MITC
time is 9/16/2003 8:28:11

Application rate (lb/acre)	Number of applications	Total Use (lb/acre/yr)	Koc (ml/g)	Soil Aerobic metabolism (days)
150.300	1.0	150.300	1.49E+01	4.8

groundwater screening cond (ppb) = 7.23E-01

EPISUITE OUTPUTS

SMILES : CNC(=S)S[Na]

CHEM : Metham sodium

CAS NUM: 000137-42-8

MOL FOR: C2 H4 N1 S2 Na1

MOL WT : 129.17

----- EPI SUMMARY (v3.10) -----

Physical Property Inputs:

Water Solubility (mg/L): -----

Vapor Pressure (mm Hg) : -----

Henry LC (atm-m³/mole) : -----

Log Kow (octanol-water): -----

Boiling Point (deg C) : -----

Melting Point (deg C) : -----

Log Octanol-Water Partition Coef (SRC):

Log Kow (KOWWIN v1.66 estimate) = -2.62

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.40):

Boiling Pt (deg C): 460.40 (Adapted Stein & Brown method)

Melting Pt (deg C): 194.10 (Mean or Weighted MP)

VP(mm Hg,25 deg C): 4.53E-009 (Modified Grain method)

Water Solubility Estimate from Log Kow (WSKOW v1.40):

Water Solubility at 25 deg C (mg/L): 1e+006

log Kow used: -2.62 (estimated)

no-melting pt equation used

Water Sol (Exper. database match) = 7.22e+005 mg/L (20 deg C)

Exper. Ref: SHIU,WY ET AL. (1990)

ECOSAR Class Program (ECOSAR v0.99g):

Class(es) found:

Neutral Organics

Henry's Law Constant (25 deg C) [HENRYWIN v3.10]:

Bond Method : Incomplete

Group Method: Incomplete

Henry's LC [VP/WSol estimate using EPI values]: 7.699E-016 atm-m³/mole

Probability of Rapid Biodegradation (BIOWIN v4.00):

Linear Model : 0.6861

Non-Linear Model : 0.7640

Expert Survey Biodegradation Results:

Ultimate Survey Model: 2.9137 (weeks)

Primary Survey Model: 3.6614 (days-weeks)

Readily Biodegradable Probability (MITI Model):

Linear Model : 0.3283

Non-Linear Model : 0.2343

Atmospheric Oxidation (25 deg C) [AopWin v1.90]:

Hydroxyl Radicals Reaction:

OVERALL OH Rate Constant = 64.2648 E-12 cm³/molecule-sec

Half-Life = 0.166 Days (12-hr day; 1.5E6 OH/cm³)

Half-Life = 1.997 Hrs

Ozone Reaction:

No Ozone Reaction Estimation

Soil Adsorption Coefficient (PCKOCWIN v1.66):

Koc : 4.038

Log Koc: 0.606

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1.67]:

Rate constants can NOT be estimated for this structure!

BCF Estimate from Log Kow (BCFWIN v2.14):

Log BCF = 0.500 (BCF = 3.162)

log Kow used: 0.48 (estimated)

Volatilization from Water:

Henry LC: 7.7E-016 atm-m³/mole (calculated from VP/WS)

Half-Life from Model River: 8.643E+011 hours (3.601E+010 days)

Half-Life from Model Lake : 9.428E+012 hours (3.928E+011 days)

Removal In Wastewater Treatment:

Total removal: 1.85 percent

Total biodegradation: 0.09 percent

Total sludge adsorption: 1.75 percent

Total to Air: 0.00 percent

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	1.3e-007	3.99	1000
Water	45.3	360	1000
Soil	54.6	360	1000
Sediment	0.0755	1.44e+003	0

Persistence Time: 421 hr

SMILES : N(=C=S)C

CHEM : Methane, isothiocyanato-

CAS NUM: 000556-61-6

MOL FOR: C2 H3 N1 S1

MOL WT : 73.11

----- EPI SUMMARY (v3.10) -----

Physical Property Inputs:

Water Solubility (mg/L): -----

Vapor Pressure (mm Hg) : -----

Henry LC (atm-m3/mole) : -----
Log Kow (octanol-water): -----
Boiling Point (deg C) : -----
Melting Point (deg C) : -----

Log Octanol-Water Partition Coef (SRC):
Log Kow (KOWWIN v1.66 estimate) = 1.30
Log Kow (Exper. database match) = 0.94
Exper. Ref: Pomona (1987)

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.40):
Boiling Pt (deg C): 90.58 (Adapted Stein & Brown method)
Melting Pt (deg C): -63.26 (Mean or Weighted MP)
VP(mm Hg,25 deg C): 12.2 (Modified Grain method)
MP (exp database): 36 deg C
BP (exp database): 119 deg C
VP (exp database): 3.54E+00 mm Hg at 25 deg C

Water Solubility Estimate from Log Kow (WSKOW v1.40):
Water Solubility at 25 deg C (mg/L): 2.113e+004
log Kow used: 0.94 (expkow database)
no-melting pt equation used
Water Sol (Exper. database match) = 7600 mg/L (20 deg C)
Exper. Ref: YALKOWSKY,SH & DANNENFELSER,RM (1992)

ECOSAR Class Program (ECOSAR v0.99g):
Class(es) found:
Thiocyanates

Henrys Law Constant (25 deg C) [HENRYWIN v3.10]:
Bond Method : 3.11E-003 atm-m3/mole
Group Method: Incomplete
Exper Database: 4.48E-05 atm-m3/mole
Henrys LC [VP/WSol estimate using EPI values]: 5.554E-005 atm-m3/mole

Probability of Rapid Biodegradation (BIOWIN v4.00):
Linear Model : 0.7127
Non-Linear Model : 0.8777

Expert Survey Biodegradation Results:
Ultimate Survey Model: 3.0376 (weeks)
Primary Survey Model: 3.7423 (days-weeks)

Readily Biodegradable Probability (MITI Model):
Linear Model : 0.4950
Non-Linear Model : 0.6069

Atmospheric Oxidation (25 deg C) [AopWin v1.90]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 0.1360 E-12 cm3/molecule-sec
Half-Life = 78.647 Days (12-hr day; 1.5E6 OH/cm3)
Ozone Reaction:
No Ozone Reaction Estimation

Soil Adsorption Coefficient (PCKOCWIN v1.66):

Koc : 3.477
Log Koc: 0.541

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1.67]:

Rate constants can NOT be estimated for this structure!

BCF Estimate from Log Kow (BCFWIN v2.14):

Log BCF = 0.500 (BCF = 3.162)
log Kow used: 0.94 (expkow database)

Volatilization from Water:

Henry LC: 4.48E-005 atm-m³/mole (Henry experimental database)

Half-Life from Model River: 12.05 hours

Half-Life from Model Lake : 203.1 hours (8.463 days)

Removal In Wastewater Treatment:

Total removal: 4.20 percent
Total biodegradation: 0.09 percent
Total sludge adsorption: 1.75 percent
Total to Air: 2.36 percent

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	15	1.89e+003	1000
Water	46.2	360	1000
Soil	38.7	360	1000
Sediment	0.0828	1.44e+003	0

Persistence Time: 274 hr

REFERENCES

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CDPR (California Dept. of Pesticide Regulation). 2002. Evaluation of Methyl Isothiocyanate as a Toxic Air Contaminant, Part A-Environmental Fate. California Environmental Protection Agency, Sacramento, CA.

EPISUITE. The EPI (Estimation Program Interface) SuiteTM is a Windows® based suite of physical/chemical property and environmental fate estimation models developed by the EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation SRC.

http://www.epa.gov/opptintr/exposure/docs/updates_episodes_v3.11.htm

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